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SPECTRAL AND SCATTERING THEORY OF SCHRÖDINGER OPERATORS AT THRESHOLDS

E. SKIBSTED

1. Rellich type theorems for atomic models

We give below an account of some of the results we presented at the Tosio Kato Centennial Conference, University of Tokyo, September 2017. They all concern versions of Rellich's theorem and appear as such as part of an ongoing project with X.P. Wang on spectral and scattering theory of N-body Schrödinger operators at two-cluster thresholds. Since the seminal paper [Re] several versions of Rellich's theorem have appeared for continuous as well as discrete Schrödinger operators, see for example the cited literature. Its combination with the Sommerfeld theorem is fundamental for stationary scattering theory, however the theorem has an interest of its own right.

1.1. **Atomic physics models.** Our main motivation are two well known models describing systems of non-relativistic charged quantum particles.

Molecules with moving nuclei:

$$H = -\sum_{j=1}^{N} \frac{1}{2m_j}\Delta_{x_j} + \sum_{1\leq i<j\leq N} q_i q_j |x_i - x_j|^{-1}, \quad x_j \in \mathbb{R}^d,\ d \geq 3, \tag{1.1}$$

where x_j, m_j and q_j denote the position, mass and charge of the j'th particle, respectively. After separating out the center of mass motion the configuration space becomes a $d(N-1)$-dimensional space $\mathbf{X}$.

Molecules with fixed nuclei: In the case of $N_c \geq 1$ infinite mass nuclei located at $R_n \in \mathbb{R}^d$, $n = 1, \dots, N_c$, the Hamiltonian reads

$$H = -\sum_{j=1}^{N} \frac{1}{2m_j}\Delta_{x_j} + \sum_{1\leq i<j\leq N} V_{ij}(x_i - x_j) + \sum_{1\leq j\leq N,\, 1\leq n\leq N_c} V_{jm}^{\mathrm{ncl}}(x_j - R_n),$$

where we impose similar conditions on V_{ij} and V_{jm}^{ncl} as in (1.1). The configuration space reads $\mathbf{X} = \mathbb{R}^{dN}$ in this case.

1.2. **Simplified presentation and notation.** For convenience of presentation let us only consider the dynamical nuclei model for which we take $d = 3$. Also we leave out completely a discussion of various generalized models of less importance in physics. We consider an arbitrary two-cluster decomposition $a_0 = (C_1, C_2)$ of the N charged particles. Suppose

$$\lambda_0 \in \sigma_{\mathrm{pp}}(H^{a_0}), \tag{1.2}$$

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and that λ_0 is not an eigenvalue of a sub-Hamiltonian H^b, where b is a cluster decomposition into at least three clusters. In other words we assume that λ_0 is a *two-cluster threshold.* The corresponding two-cluster decomposition a_0 may be unique or non-unique. But for any such $a_0 = (C_1, C_2)$ we can introduce *cluster charges*

$$Q_1 = \sum_{j \in C_1} q_j \text{ and } Q_2 = \sum_{j \in C_2} q_j.$$

If ϕ_j, $j = 1, 2$, denote cluster bound states, $(H^{C_j} - \lambda_j)\phi_j = 0$, and $\lambda_1 + \lambda_2 = \lambda_0$, then $\phi_0 = \phi_1 \otimes \phi_2$ is a bound state corresponding to (1.2). Writing $H = H^{a_0} \otimes I + I_{a_0}$ the effective interaction between the clusters is the partial inner product $\langle \phi_0, I_{a_0}\phi_0 \rangle_{L^2(\mathbf{X}^{a_0})}$, which is a function of the inter-cluster coordinate x_{a_0} only. It has a long-range behaviour if $Q_1 Q_2 \neq 0$. Otherwise it may have order $|x_{a_0}|^{-2}$ behaviour at infinity or, as an alternative, it is $O(|x_{a_0}|^{-3})$; this depends on the cluster charges and in addition on *cluster charge moments.* The detailed analysis of the structure of bound and resonance states for the full Hamiltonian H at λ_0 depends on the asymptotics of this effective interaction.

1.3. **Rellich type theorems.** Let us first recall a version of Rellich's theorem away from thresholds, cf. [Is, IS]. It is here stated in terms of weighted L^2-spaces $L^2_s = L^2_s(\mathbf{X}) = \langle x \rangle^{-s} L^2$, $s \in \mathbb{R}$, although there exists a more refined Besov space version. We introduce for $s \geq 0$ and $\lambda \in \mathbb{R}$ the space

$$\mathcal{E}_{-s}(\lambda) = \{\phi \in L^2_{-s} \quad | \quad (H - \lambda)\phi = 0\}.$$

Theorem 1.1 (non-threshold version of Rellich's theorem). *Suppose λ is <u>not</u> a threshold. Then for $s = 1/2$*

$$\dim \mathcal{E}_{-s}(\lambda) < \infty \textit{ and } \mathcal{E}_{-s}(\lambda) \subseteq L^2_\infty \; (:= \cap_t L^2_t).$$

A general result for two-cluster thresholds is the following.

Theorem 1.2 (Rellich's theorem for a general two-cluster threshold). *For any two-cluster threshold λ_0 and for $s = 1/2$*

$$\dim \mathcal{E}_{-s}(\lambda_0) < \infty. \tag{1.3}$$

The proofs of these theorems are very different. The proof of the first result uses the Mourre estimate, while the proof of the second result is based on Fredholm theory. Behind the latter result there is more detailed information depending on relevant cluster charges and cluster charge moments. We shall not here elaborate on the general case. Rather we confine ourselves to stating such more detailed information in a special case, more precisely for the lowest threshold $\Sigma_2 := \min \sigma_{\text{ess}}(H)$.

Theorem 1.3 (Rellich's theorem for the lowest threshold). *Suppose $\lambda_0 = \Sigma_2$ is a two-cluster threshold. Then* (1.3) *is fulfilled for $s = 3/4$. More precisely, depending on charge/charge moment relations there are four cases (if the two-cluster decomposition $a_0 = (C_1, C_2)$ is non-unique we assume these cases to hold uniformly in a_0):*

1) *($Q_1Q_2 < 0$; effective attractive Coulomb interaction) For $s = 3/4$*

$$\dim \mathcal{E}_{-s}(\lambda_0) < \infty.$$

Moreover (arbitrary polynomial decay) $\mathcal{E}_{-3/4}(\lambda_0) \subseteq L^2_\infty$.

2) *($Q_1Q_2 > 0$; effective repulsive Coulomb interaction) For all $s \geq 0$*

$$\dim \mathcal{E}_{-s}(\lambda_0) < \infty \text{ and } \mathcal{E}_{-s}(\lambda_0) \subseteq L^2_\infty.$$

3) *($Q_1Q_2 = 0$; effective $O(r^{-2})$ interaction) For a 'computable' $s_0 \geq 1$*

$$\dim \mathcal{E}_{-s_0}(\lambda_0) < \infty.$$

There is a 'computable' $d_0 \in \mathbb{N}$ such that $\dim\left(\mathcal{E}_{-s}(\lambda_0)/L^2\right) \leq d_0$ for all $s < s_0$.

4) *($Q_1Q_2 = 0$; effective $O(r^{-3})$ interaction) The dimension*

$$\dim \mathcal{E}_{-3/2}(\lambda_0) < \infty.$$

Moreover

$$\dim\left(\mathcal{E}_{-3/2}(\lambda_0)/L^2\right) \leq \sum_{\textit{two-clusters},\, \#a=2} \dim \ker(H^a - \lambda_0).$$

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(E. Skibsted) Institut for Matematiske Fag, Aarhus Universitet, Ny Munkegade 8000 Aarhus C, Denmark

E-mail address: skibsted@math.au.dk